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A MODIFIED BENEDICT–WEBB–RUBIN EQUATION OF STATE FOR GASEOUS AND LIQUID OXYGEN

L. A. Weber

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Cryogenics Division
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Boulder,Colorado 80303

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Prepared for

NASA-Johnson Space Center
Houston, Texas 77058

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Contents

		Page
1.	Introduction	1
2.	The Data	2
3.	The Equation of State for Oxygen	4
4.	Auxiliary Information	6
	4.1. Two-Phase Boundaries	6
	4.2. Vapor Pressure Curve	6
	4.3. Saturation Densities	7
	4.4. Melting Pressures	8
	4.5. Ideal Gas Thermodynamic Properties	8
	4.6. Summary of Fixed Points for Oxygen	8
5.	The Properties Deck	10
6.	Quality of the Fit and Accuracy of the Derived Properties	10
	6.1. Density Deviations	10
	6.2. Comparison of Derived Thermodynamic Properties	11
7.	Summary	12
8.	References	31
Appendix A		13
Appendix B		26

List of Figures

Figure 1. Deviations of the density data from eqn. (1) on several isotherms 27

Figure 2. Deviations of the saturation densities from the values calculated via eqn. (1); O - liquid, O - vapor 28

Figure 3. Deviations of the heat capacity data on three isochores from values calculated by eqn. (1) 29

Figure 4. Deviations of the velocity of sound data from values calculated via the equation of state on several isotherms . . 30

List of Tables

Page

Table 1. Data Used to Determine the Parameters of the Equation of State 3

Table 2. Coefficients for the Equation of State (1) 5

Table 3. Parameter Values for the Various Equations 9

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New PVT data on oxygen at pressures to 800 atmospheres have been recently reported. These data, along with other NBS data on oxygen have been fitted with a 32 term modified Benedict-Webb-Rubin equation of state. This equation is valid for gaseous and liquid oxygen at temperatures from the triple point (54.36 K) to 300 K and for pressures up to 800 atm. Thermophysical properties calculated via this equation are compared with the most reliable values available. The vapor pressure equation has also been updated to be consistent with more recent experimental work near the triple point. A computer program is available which calculates the thermophysical properties of oxygen.

Key words: Density; enthalpy; entropy; equation of state; oxygen; oxygen property computer program; PVT; saturation properties; specific heat.

1. Introduction

A modified form of the Benedict-Webb-Rubin (BWR) equation of state [1], with more terms added, is often the most convenient way of representing the PVT surface of a fluid and of calculating its thermodynamic properties. Recent versions, such as the thirty-two term modification of Jacobsen [2], also fit PVT data with deviations no larger than the experimental uncertainty over most of the PVT surface.

The fact that many of the derived thermodynamic properties can be calculated explicitly in closed, analytic form greatly enhances the usefulness of the equation

and the speed of machine calculations. This characteristic of the equation also allows it to be fit to several properties simultaneously (e.g., density and specific heat). Such multi-property fitting virtually assures the accuracy of most derived thermodynamic properties, provided sufficient good data are available.

In an earlier report, Roder and McCarty [10] described the application of the 32 term version of the equation to the data on parahydrogen. This report describes the fitting of the equation to the NBS data on oxygen. Stewart and Jacobsen [2,6] have successfully applied this equation to oxygen. However, the availability of significant new PVT data [4] justifies the refitting described here.

We have changed slightly the vapor pressure equation used previously, and the equation with the new parameters is repeated here. Also repeated here are the representations used previously for the densities of saturated liquid and vapor and for the melting pressure as functions of temperature.

2. The Data

All of the data used for fitting the equation came from this laboratory. These comprise the bulk of all the data available for oxygen, and provide us with a data set having a high degree of internal consistency. The data used comprise a close-spaced set of 2064 points, summarized in table 1. The experimental details are given in refs [3,4,5]. With the exception of some critical region measurements from [11], the saturation boundary data are not independent experimental data but were derived from the intersection of the single-phase experimental isochores with the vapor pressure curve. The resulting points were smoothed and interpolated by means of the function given in section 4.3, and the smoothed data were used in the equation of state fitting. The Gibbs constraints are not actually constraints but rather calculated data setting the Gibbs free energy of the coexisting liquid and vapor states equal at a given temperature.

The earlier PVT data of [3] were not reported on the currently accepted International Practical Temperature Scale of 1968 (T_{68}), and thus it was necessary to convert them to this scale by means of the conversion tables given in Metrologia [7].

Table 1. Data Used to Determine the Parameters of the Equation of State.

Type of Data	No. Points	Range		Source
		T(K)	P(atm)	
PVT	1435	56 - 300	2 - 340	Weber [3]
PVT	348	56 - 300	50 - 800	Weber [4]
Saturation Boundary	100	56 - 154	0.002 - 49	Weber [3]
C_v	131	58 - 284	42 - 284	Goodwin & Weber [5]
Gibbs Constraint	50	56 - 154	0.002 - 49	Weber [3]

3. The Equation of State for Oxygen

The original Benedict-Webb-Rubin equation of state [1] was modified by Strobridge [8] in 1962. Strobridge's equation contained 16 terms, and it was adequate for the data then available for nitrogen. However, when Roder and Goodwin [9] applied it to a close-spaced, high precision data set for parahydrogen they were forced to divide the PVT surface into liquid and gaseous regions and use two sets of parameters in order to fit the experimental data. They were unable to eliminate discrepancies in the derived properties at the junction of the two surfaces. Since 1974 McCarty [10] has applied the 32 term version of Jacobsen [2] to several cryogenic fluids. The resulting "single surface" representations reproduced the data very well except in the critical region where no analytic representation can be expected to show proper behavior. This version was therefore chosen to represent the data for oxygen. The equation of state is:

$$
\begin{aligned}
P = \rho RT &+ \rho^2 (A_1 T + A_2 T^{1/2} + A_3 + A_4/T + A_5/T^2) \\
&+ \rho^3 (A_6 T + A_7 + A_8/T + A_9/T^2) \\
&+ \rho^4 (A_{10} T + A_{11} + A_{12}/T) + \rho^5 (A_{13}) \\
&+ \rho^6 (A_{14}/T + A_{15}/T^2) + \rho^7 (A_{16}/T) \\
&+ \rho^8 (A_{17}/T + A_{18}/T^2) + \rho^9 (A_{19}/T^2) \\
&+ e^{-\gamma\rho^2} \Big[\rho^3 (A_{20}/T^2 + A_{21}/T^3) + \rho^5 (A_{22}/T^2 + A_{23}/T^4) \\
&\qquad + \rho^7 (A_{24}/T^2 + A_{25}/T^3) \\
&\qquad + \rho^9 (A_{26}/T^2 + A_{27}/T^4) \\
&\qquad + \rho^{11} (A_{28}/T^2 + A_{29}/T^3) \\
&\qquad + \rho^{13} (A_{30}/T^2 + A_{31}/T^3 + A_{32}/T^4) \Big]
\end{aligned}
\tag{1}
$$

Table 2. Coefficients for the Equation of State (1).

$R = 0.08205616$ L atm/mol K $\qquad \gamma = -0.0056$

G(1)	=	-.4308768468E-03
G(2)	=	.1979591095E+00
G(3)	=	-.4143014968E+01
G(4)	=	.1853654396E+03
G(5)	=	-.1270637452E+05
G(6)	=	.1536388737E-04
G(7)	=	.1326068945E-02
G(8)	=	-.2199275123E+01
G(9)	=	.4705445127E+04
G(10)	=	.4728198017E-06
G(11)	=	.2430408198E-02
G(12)	=	-.1896759615E+00
G(13)	=	-.6887067207E-05
G(14)	=	-.6132885180E-03
G(15)	=	-.1836518694E+00
G(16)	=	.2575663871E-04
G(17)	=	-.2415604646E-06
G(18)	=	.1438680831E-03
G(19)	=	-.1703915986E-05
G(20)	=	-.2353705917E+04
G(21)	=	-.2271707669E+06
G(22)	=	-.2753815471E+02
G(23)	=	.9277648729E+05
G(24)	=	-.4114926856E-01
G(25)	=	.1982233262E+01
G(26)	=	-.1239651142E-03
G(27)	=	-.6322588664E+00
G(28)	=	-.2443207666E-07
G(29)	=	.1328704370E-04
G(30)	=	-.1146313812E-09
G(31)	=	-.1021169305E-07
G(32)	=	.2334998237E-06

The coefficients, given in table 2, were found by least square fitting eq (1) to the data set in table 1, with the density, ρ, in mols/liter, pressure, P, in atmospheres, and the temperature, T, in Kelvins.

In the fitting procedure each data point was weighted according to a scheme which utilized the estimated uncertainties in the experimental quantities. In addition, three constraints were imposed on the equation. At the critical point, the density was constrained to be equal to ρ_c; also the derivatives $(\partial P/\partial\rho)_T$ and $(\partial^2 P/\partial\rho^2)_T$ were constrained to be equal to zero. The critical point used was the one determined previously [11]: ρ_c = 13.63 mol/L, T_c = 154.581 K, and P_c = 49.768 atm.

4. Auxiliary Information

4.1. Two-Phase Boundaries

The equation of state representation of the previous section does not recognize the existence of phase boundaries, and these must be specified independently to complete the description of the PVT surface. The liquid-vapor two phase region can be inferred from van der Waals type "loops" in the isotherms of the equation of state surface at subcritical temperatures. A liquid-vapor two phase boundary (saturation boundary) can be calculated from the equation of state surface by setting equal the Gibbs free energy of the liquid and vapor states at a given temperature. The vapor pressure thus derived generally agrees with the true vapor pressure to within 0.1 - 0.2 percent. However, the results are generally more accurate if we specify the vapor pressure curve independently.

4.2. Vapor Pressure Curve

Although a polynomial representation of the vapor pressure can be made sufficiently accurate for most purposes, the formulation given by Goodwin [12] has many advantages:

$$\ell n\left(\frac{P}{P_t}\right) = A\chi + B\chi^2 + C\chi^3 + D\chi(1-\chi)^{\varepsilon}, \qquad (2)$$

where $\chi = (1 - T_t/T)/(1 - T_t/T_c)$, and P_t and T_t are the triple point pressure and temperature. This equation has the proper limiting form ($\ell nP \sim a + b/T$) at

low pressures near the triple point. It has the proper non-analytic form to fit data near the critical point, and it fits the data with fewer parameters than a polynomial. The parameters have similar values for all cryogenic fluids, and the exponent, ε, is close enough to the value 3/2 that it is sometimes considered a "universal parameter" for this class of substances. If the triple point pressure is known, eq (2) is constrained to that value; otherwise it may be used as a variable parameter. The parameter values used in eq (2) are given in table 3.

4.3. Saturation Densities

Given the vapor pressure curve, saturation densities can be calculated via the equation of state (1). It is sometimes convenient, however, to have an explicit formulation of the densities of the saturated liquid and vapor. They may be expressed by

$$\rho_{SAT}\ (\text{liquid}) = \rho_{RD} + f(T) \tag{3a}$$

$$\rho_{SAT}\ (\text{vapor}) = \rho_{RD} - f(T) \tag{3b}$$

where the rectilinear diameter, ρ_{RD}, (defined by $\rho_{RD} = \frac{1}{2}\ [\rho_{SAT}\ (\text{liquid}) + \rho_{SAT}\ (\text{vapor})]$, is

$$\rho_{RD} = \rho_c + a_1(T_c - T) + a_2(T_c - T)^2 \tag{4}$$

and

$$f(T) = \rho_c \sum_{J=1}^{3} A_J \left(\frac{T_c - T}{T_c}\right)^{(2J - 1)\beta} . \tag{5}$$

The parameter values are given in table 3. With the parameters given, eqs (3-5) should only be used in the temperature range 120 K to T_c = 154.581 K.

4.4. Melting Pressures

The melting pressure data from [3] and [13] are accurately represented by the equation

$$P = P_t + P_o [(T/T_t)^c - 1] \quad (6)$$

up to a pressure of 3500 atm. Parameter values are given in table 3.

4.5. Ideal Gas Thermodynamic Properties

By means of the relationships given in [3], equation (1) can be used to calculate changes in thermodynamic properties along any isothermal path, including those passing through the liquid-vapor two phase region. In order to relate property values at different temperatures, we must add to these changes the values of the thermodynamic properties in the ideal gas state at that temperature. The latter are easily calculated via the relationship used for the ideal gas specific heat

$$\frac{C_p^o(T)}{R} = \sum_{J=1}^{7} A_J T^{(J-4)} + A_8 \frac{u^2 e^u}{(e^u - 1)^2} \quad (7)$$

where $u = A_9/T$. Parameter values are given in table 3. From eqs (1) and (7) and the values of the enthalpy and entropy in the ideal gas state at one temperature, all of the thermodynamic properties of the fluid may be calculated at any temperature and pressure. For the reference state we have chosen the values at T = 298.15 K, P = 1 atm,

$$H^\circ = 8682 \text{ J/mol}$$
$$S^\circ = 205.037 \text{ J/mol-K}$$

from CODATA [14].

4.6. Summary of Fixed Points for Oxygen

In this report the following values have been specified as fixed; the subscripts t, b, and c refer to the triple, boiling, and critical points respectively.

Table 3. Parameter Values for the Various Equations.

Vapor pressure, eq (2):

$A = 7.797\ 7723$ $\quad D = 3.293\ 8576$

$B = 4.577\ 3000$ $\quad \varepsilon = 1.5$

$C = -1.928\ 1264$

Saturation densities, eqs (4) and (5):

$a_1 = 6.0402 \times 10^{-5}$ $\quad a_2 = 9.80 \times 10^{-8}$

$A_1 = 1.811\ 3127$ $\quad A_3 = -7.580\ 9408 \times 10^{-1}$

$A_2 = 2.775\ 1793 \times 10^{-1}$ $\quad \beta = 0.353$

Melting pressure, eq (6):

$P_o = 2637.3$ atm $\quad c = 1.769$

$P_t = 0.0014451$ atm $\quad T_t = 54.359$ K

Ideal gas specific heat, eq (7):

$A_1 = -1.86442361 \times 10^{2}$ $\quad A_6 = -1.11035799 \times 10^{-8}$

$A_2 = 2.0784024 \times 10$ $\quad A_7 = 2.08612876 \times 10^{-11}$

$A_3 = -3.42642911 \times 10^{-1}$ $\quad A_8 = 1.01894691$

$A_4 = 3.50297163$ $\quad A_9 = 2.23918105 \times 10^{3}$

$A_5 = 2.05866482 \times 10^{-7}$

Triple Point:	T_t	= 54.359 K
	P_t	= 0.0014451 atm
Boiling Point:	T_b	= 90.188 K
	P_b	= 1.0 atm
Critical Point:	T_c	= 154.581 K
	P_c	= 49.768 atm
	ρ_c	= 13.63 mol/L

5. The Properties Deck

In the appendix is a listing of a set of subroutines useful for utilizing the foregoing relationships to calculate the thermophysical properties of oxygen. This properties deck was developed by R. D. McCarty [15] for use on the Control Data Corporation 6600 computer, and it is available from the NBS Cryogenic Data Center, Boulder, Colorado. A listing of the deck is given in Appendix A, and a test program and sample results are in Appendix B.

6. Quality of the Fit and Accuracy of the Derived Properties

Because of the wealth of consistent data available for oxygen, this report provides a good indication of the ability of the 32 term modified BWR equation to fit the PVT surface of a classical gas and to provide accurate derived properties. The following sections provide enough comparisons with experimental data to show the general quality of the fit and to indicate regions of difficulty.

6.1. Density Deviations

In fig 1 are shown deviations of the density data from the calculated surface at eight temperatures, 70, 120, 140, 150, 156, 170, 200, and 300 K. Overall we see that the equation reproduces the data very well. This is especially true in the compressed liquid. Only in the region of the critical point does the equation fail to reproduce the PVT surface accurately. The deviation plot for the 156 K isotherm, and to a lesser extent the 170 K isotherm, are typical of the inability of an analytic equation of state to fit PVT data in the critical region. Neglecting those points, however, the average deviation of the equation from the data is about 0.04 percent in density. This amount is about twice the imprecision in the data, but it is less than the overall uncertainty in the data of about 0.1%, due to possible systematic errors.

Deviations of the calculated saturation densities are given in fig 2. Here again it is seen that the deviations are larger in the critical region. They become smaller in the immediate vicinity of the critical point, however, because the equation is constrained at that point.

6.2. Comparison of Derived Thermodynamic Properties

(a) Specific heat at constant volume: Goodwin and Weber [5] measured C_v for oxygen at eighteen different densities. One, apparently spurious, set of data at a density of 5.1 mol/L was discarded, as were several data near critical, and the rest were incorporated in the data set used for determining the equation of state. These data had a reproducibility of about 0.25 percent. The average difference between the calculated and experimental values was 0.67 percent, approximately equal to the overall uncertainty of the data as expressed in [5]. The maximum deviation for the data used in the fit, 4.2 percent, occurred at 162 K near the critical density. Calculated values deviated from several other near critical experimental points, not used in the fit, by as much as 20 percent. This behavior is typical for an analytic equation of state near the critical point. Deviations of the calculated C_v's from the experimental data at three densities are shown in fig 3.

(b) Velocity of sound. Extensive measurements of the velocity of sound in oxygen have been reported by van Itterbeek and van Dael [16] and by Straty and Younglove [17]. Experimental pressures ranged as high as 900 atm in the compressed liquid and 350 atm for the high temperature gas. These data have an experimental uncertainty of 0.1 percent or less. Therefore, although they cannot be readily incorporated into the multiproperty fitting techniques, they do provide a sensitive test of the quality of the calculated PVT surface.

The data of van Itterbeek and van Dael are on five isotherms from 67.5 to 90.4 K at pressures to 900 atm. The calculated velocities are generally smaller than the experimental ones by a little over one percent, with the maximum deviation being 2.0 percent. Comparison with the data of Straty and Younglove indicates that the calculated values are again smaller, the difference averaging about 1.4 percent in the compressed liquid and decreasing to about 0.4 percent at supercritical temperatures. The deviations on several isotherms are shown in fig 4.

(c) Other thermodynamic properties. Other properties such as entropy, enthalpy, etc. could be used in the multi-property fitting process. However, no experimental measurements exist for these properties of oxygen. Instead we have compared values calculated via the BWR equation with values calculated in ref [4], which used a different type of surface representation.

A spot check of the calculated entropies at 60, 100, 200 and 300 K and pressures from 50 to 1000 atm showed differences ranging from 0.03 to 0.12 J/mol-K. This agreement is quite good and is within the estimates of accuracy in [4]. The maximum differences might be expected to occur at the critical point, and here the two methods disagree by only 0.3 J/mol-K. A similar comparison for enthalpy showed agreement generally within $\pm$ 7 J/mol.

At the liquid-vapor two phase boundary, the Gibbs "constraint," which sets

$$G_g - G_\ell = \Delta G = \Delta H - T\Delta S = 0 \ ,$$

was satisfied to within 1-3 J/mol at all temperatures from 56 to 154 K.

In the critical region, which for present purposes we may define as $\pm$ 0.25 ρ_c at the critical temperature and extending out 20 K above T_c at the critical density, the isothermal compressibility, $(\partial\rho/\partial P)_T/\rho$, is subject to large errors. For this reason values of the specific heat C_p should be considered unreliable in this region.

7. Summary

A total of 2064 data points for oxygen, including PVT, C_v, and Gibbs free energy data, have been fit with a 32 term modified Benedict-Webb-Rubin equation of state. The equation represents the data very well in all regions except near the critical point. The equation is valid over the whole range of the data from the triple point (54.36 K) to 300 K and to pressures of 1000 atm, but it should not be extrapolated beyond this range without caution. It allows calculation of the derived thermodynamic properties with an accuracy equal to that with which they are known, with the possible exception of the sound velocities at high densities. Even the latter are calculated with an accuracy sufficient for most purposes.

```
      SUBROUTINE DATA 02
      DIMENSION G(32),VP(9),GI(11)
      DIMENSION GV(9),GT(9),FV(4),FT(4),EV(8),ET(8)
      COMMON/DATA1/GV,GT,FV,FT,EV,ET
      COMMON/SEN/BETA,XO,DELTA,E1, E2, AGAM
      COMMON/CRIT/ EM, EOK, RM, TC, DC, X , PC, SIG
      COMMON/DATA/G,R,GAMMA,VP,DTP
      COMMON/ISP/N,NW,NWW
      COMMON/CPID/GI
      NWW=0
      N=0 $ NW=1
       XO=0.183   $ BETA=0.355 $ DELTA=4.352 $ E1=2.21 $ E2=0.287
       EM=31.9988 $ EOK=113.0 $ RM=3.8896E-08$ TC=154.575
       DC=0.4362 $ X=2.210636 $ PC=49.770 $ SIG=3.437
      AGAM = 1.190
C     TRANSPORT PROPERTIES
CC    FROM HANLEY ET. AL.
C     VOL 3, NO 4, 1974
      GV(1)=-9.7076378593E+1   $  GV(2)=8.2801254201E+1
      GV(3)=-2.4668758803E+1 $ GV(4)=2.1324360243
      GV(5)=3.7851049522E-1   $  GV(6)=-1.0487216090E-1
      GV(7)=1.1134441304E-2   $  GV(8)=-5.3676093757E-4
      GV(9)=1.0279379641E-5
      GT(1)=-2.0395052193E+5   $  GT(2)=2.4088141709E+5
      GT(3)=-1.2014175183E+5   $  GT(4)=3.295494919E+4
      GT(5)=-5.4244239598E+3   $  GT(6)=5.4734865540E+2
      GT(7)=-3.2854821539E+1   $  GT(8)=1.0753572103
      GT(9)=-1.4610986820E-2
      EV(1)=-1.2152387017E+1   $  EV(2)=-3.1421728994E-1
      EV(3)=1.8201161468E+1   $  EV(4)=2.7390429525E+2
      EV(5)=-2.7498956948E+3   $  EV(6)=2.4340689667E+2
      EV(7)=1.1911504104E+2 $  EV(8)=.435
       FV(1)=4.3526515153 $ FV(2)= -2.0361263878
      FV(3)=1.4   $  FV(4)=100.
      FT(1)=.3060       $FT(2)=.2785
      FT(3)=1.12   $  FT(4)=100.
      ET(1)=-1.2310400765E+1   $  ET(2)=1.6799504261E+1
      ET(3)=-2.9944878721E+3   $  ET(4)=4.7350508788E+2
C     THERMODYNAMIC PROPERTIES
CC    FROM WEBER - TO BE PUBLISHED
      R=8.205616E-2
      GAMMA=-.0056
       GI(1)=    -0.498199853711943E 04
       GI(2)=     0.230247779995218E 03
       GI(3)=    -0.345565323510732E 01
       GI(4)=     0.352187677367116E 01
       GI(5)=    -0.435420216024420E-04
       GI(6)=     0.134635345013162E-07
       GI(7)=     0.162059825959105E-10
       GI(8)=     0.103146851572565E 01
      GI(9)=     0.2239181050000000E 04
      GI(10)=GI(11)=0
      TO=298.15   $  HO=8682.   $  SO=205.037
      GI(10)=HO-HI(TO)
      GI(11)=SO-SI(TO)
      G(1)=    -.4308768468E-03
      G(2)=     .1979591095E+00
      G(3)=    -.4143014968E+01
      G(4)=     .1853654396E+03
      G(5)=    -.1270637452E+05
      G(6)=     .1536388737E-04
      G(7)=     .1326068945E-02
      G(8)=    -.2199275123E+01
      G(9)=     .4705445127E+04
      G(10)=    .4728198017E-06
      G(11)=    .2430408198E-02
      G(12)=   -.1896759615E+00
      G(13)=   -.6887067207E-05
      G(14)=   -.6132885180E-03
      G(15)=   -.1836518694E+00
      G(16)=    .2575663871E-04
      G(17)=   -.2415604646E-06
      G(18)=    .1438680831E-03
      G(19)=   -.1703915986E-05
      G(20)=   -.2353705917E+04
      G(21)=   -.2271707669E+06
      G(22)=   -.2753815471E+02
      G(23)=    .9277648729E+05
      G(24)=   -.4114926856E-01
```

```
      G(25)=    .1982233262E+01
      G(26)=   -.1239651142E-03
      G(27)=   -.6322588664E+00
      G(28)=   -.2443207666E-07
      G(29)=    .1328704370E-04
      G(30)=   -.1146313812E-09
      G(31)=   -.1021169305E-07
      G(32)=    .2334998237E-06
      VP(1)=7.7977723 $ VP(2)=4.57730 $ VP(3)=-1.9281264
      VP(4)=3.2931232 $ VP(5)=1.5 $ VP(6)=0.0014451
      VP(7)=54.359   $  VP(8)=154.581
      VP(9)=0.0
      DTP=40.84
      RETURN   $  END



      FUNCTION VPN(TT)
C     CALCULATES VAPOR PRESSURE IN ATMOSPHERES
C     FOR AN INPUT TEMPERATURE IN KELVIN
      DIMENSION G(32),VP(9)
      COMMON/DATA/G,R,GAMMA,VP
      T=TT
      X=(1.-VP(7)/T)/(1.-VP(7)/VP(8))
      VPN=VP(6)*EXP (VP(1)*X+VP(2)*X*X+VP(3)*X**3+VP(9)*X**4+VP(4)*X*
     1(1.-X)**VP(5))
      RETURN
      END



      FUNCTION DPDTVP(TT)
C     CALCULATES THE DERIVATIVE OF PRESSURE
C     WITH RESPECT TO TEMPERATURE AT
C     SATURATION.  INPUT IS TEMP. IN K, OUTPUT IS ATM/K.
      COMMON/DATA/G,R,GAMMA,VP
      DIMENSION G(32),VP(9)
      T=TT
      IF(TT.GT.VP(8))GO TO 1
      X=(1.-VP(7)/T)/(1.-VP(7)/VP(8))
      DXDT=(VP(7)/T**2)/(1.-VP(7)/VP(8))
      DPDT=VP(1)*DXDT+2.*VP(2)*X*DXDT+VP(3)*3.*X**2*DXDT+VP(4)*
     1((1.-X)**VP(5))*DXDT+VP(4)*X*((1.-X)**(VP(5)-1.))*VP(5)*(-DXDT)
      DPDT=DPDT*VPN(T)
      DPDTVP=DPDT
      RETURN
    1 DPDTVP=0
      RETURN
      END



      FUNCTION FINDTV(POBS)
C     ITTERATES THE VAPOR PRESSURE EQUATION
C     FOR A TEMPERATURE ( IN KELVIN)
C     GIVEN AN INPUT PRESSURE IN ATMOSPHERES
      COMMON/DATA/G,R,GAMMA,VP,DTP
      DIMENSION G(32),VP(9)
      T=(VP(7)+VP(8))/2.
      DO 7 I=1,10
      P=VPN(T)
      IF(ABS (P-POBS)-.000001*POBS)8,8,6
    6 CONTINUE
      CORR=(POBS-P)/DPDTVP(T)
    7 T=T+CORR
    8 CONTINUE
      FINDTV=T
      RETURN
      END
```

```
      SUBROUTINE PROPS(PP,DD,TT)
      DIMENSION X(33)
      DIMENSION B(33),G(32)
      EQUIVALENCE (B,X)
      COMMON/DATA/G,R,GAMMA
      COMMON/1/B
      DATA(ID=1)
      DATA(IZ=1)
    1 CONTINUE
      IF(IZ.LE.0)GO TO 2
      IZ=0
    2 CONTINUE
      D=DD
      P=PP
      T=TT
      GM=GAMMA
      D2=D*D
      D3=D2*D
      D4=D3*D
      D5=D4*D
      D6=D5*D
      D7=D6*D
      D8=D7*D
      D9=D8*D
      D10=D9*D
      D11=D10*D
      D12=D11*D
      D13=D12*D
      TS=SQRT (T)
      T2=T*T
      T3=T2*T
      T4=T3*T
      T5=T4*T
      F=EXP (GM*D2)
      GO TO (100,200,300,400,500,600,700),K
      ENTRY PRESS
C     ENTRY FOR PRESSURE, INPUT IS DENSITY
C     AND TEMP. IN MOL/L AND K, OUTPUT IS IN ATM.
      K=1
      GO TO 1
  100 CONTINUE
      B( 1)=D2*T
      B( 2)=D2*TS
      B( 3)=D2
      B( 4)=D2/T
      B( 5)=D2/T2
      B( 6)=D3*T
      B( 7)=D3
      B( 8)=D3/T
      B( 9)=D3/T2
      B(10)=D4*T
      B(11)=D4
      B(12)=D4/T
      B(13)=D5
      B(14)=D6/T
      B(15)=D6/T2
      B(16)=D7/T
      B(17)=D8/T
      B(18)=D8/T2
      B(19)=D9/T2
      B(20)=D3*F/T2
      B(21)=D3*F/T3
      B(22)=D5*F/T2
      B(23)=D5*F/T4
      B(24)=D7*F/T2
      B(25)=D7*F/T3
      B(26)=D9*F/T2
      B(27)=D9*F/T4
      B(28)=D11*F/T2
      B(29)=D11*F/T3
      B(30)=D13*F/T2
      B(31)=D13*F/T3
      B(32)=D13*F/T4
      IF(ID.GT.0)GO TO 102
      B(33)=P-R*D*T
      RETURN
  102 P=0
      M=32
      DO 101 I=1,M
```

```
  101 P=P+B(I)*G(I)
      P=P+R*D*T
      PP=P
      RETURN
      ENTRY DPDD
C     PARTIAL OF PRESSURE WITH RESPECT TO
C     DENSITY - SEE PRESSURE
C     ENTRY FOR UNITS
      K=2
      GO TO 1
  200 CONTINUE
      F1=2.00*F*GM*D
      F21=3.000*F*D2 +F1*D3
      F22=5.000*F*D4 +F1*D5
      F23=7.000*F*D6 +F1*D7
      F24=9.000*F*D8 +F1*D9
      F25=11.00*F*D10+F1*D11
      F26=13.00*F*D12+F1*D13
      B( 1)=2.00*D*T
      B( 2)=2.00*D*TS
      B( 3)=2.00*D
      B( 4)=2.00*D/T
      B( 5)=2.00*D/T2
      B( 6)=3.00*D2*T
      B( 7)=3.00*D2
      B( 8)=3.00*D2/T
      B( 9)=3.00*D2/T2
      B(10)=4.00*D3*T
      B(11)=4.00*D3
      B(12)=4.00*D3/T
      B(13)=5.00*D4
      B(14)=6.00*D5/T
      B(15)=6.00*D5/T2
      B(16)=7.00*D6/T
      B(17)=8.00*D7/T
      B(18)=8.00*D7/T2
      B(19)=9.00*D8/T2
      B(20)=F21/T2
      B(21)=F21/T3
      B(22)=F22/T2
      B(23)=F22/T4
      B(24)=F23/T2
      B(25)=F23/T3
      B(26)=F24/T2
      B(27)=F24/T4
      B(28)=F25/T2
      B(29)=F25/T3
      B(30)=F26/T2
      B(31)=F26/T3
      B(32)=F26/T4
      M=32
      IF(ID.GT.0)GO TO 202
      B(33)=P-R*T
      RETURN
  202 P=0
      DO 201 I=1,M
  201 P=P+B(I)*G(I)
      P=P+R*T
      PP=P
      RETURN
      ENTRY DPDT
C     PARTIAL OF PRESSURE WITH RESPECT
C     TO TEMPERATURE - SEE PRESSURE
C     ENTRY FOR UNITS
      K=3
      GO TO 1
  300 CONTINUE
      X( 1)=D2
      X( 2)=D2/(2.00*TS)
      X( 3)=0
      X( 4)=-D2/T2
      X( 5)=-2.00*D2/T3
      X( 6)=D3
      X( 7)=0
      X( 8)=-D3/T2
      X( 9)=-2.00*D3/T3
      X(10)=D4
      X(11)=0
      X(12)=-D4/T2
```

```
      X(13)=0
      X(14)=-D6/T2
      X(15)=-2.00*D6/T3
      X(16)=-D7/T2
      X(17)=-D8/T2
      X(18)=-2.00*D8/T3
      X(19)=-2.00*D9/T3
      X(20)=-2.00*D3*F/T3
      X(21)=-3.00*D3*F/T4
      X(22)=-2.00*D5*F/T3
      X(23)=-4.00*D5*F/T5
      X(24)=-2.00*D7*F/T3
      X(25)=-3.00*D7*F/T4
      X(26)=-2.00*D9*F/T3
      X(27)=-4.00*D9*F/T5
      X(28)=-2.00*D11*F/T3
      X(29)=-3.00*D11*F/T4
      X(30)=-2.00*D13*F/T3
      X(31)=-3.00*D13*F/T4
      X(32)=-4.00*D13*F/T5
      IF(ID.GT.0)GO TO 302
      X(33)=PP-R*D
      RETURN
  302 P=0
      DO 301 I=1,32
  301 P=P+G(I)*X(I)
      PP=P+R*D
      RETURN
      ENTRY DSDN
C     PARTIAL OF ENTROPY WITH
C     RESPECT TO THE G COEFFICIENTS
      K=4
      GO TO 1
  400 CONTINUE
C     S=S0-R*LOGF(D*R*T/P0)+(DSDN(D)-DSDN(0))*101.325 +CPOS(T)
      G1=F/(2.00*GM)
      G2=(F*D2-2.00*G1)/(2.00*GM)
      G3=(F*D4-4.00*G2)/(2.00*GM)
      G4=(F*D6-6.00*G3)/(2.00*GM)
      G5=(F*D8-8.00*G4)/(2.00*GM)
      G6=(F*D10-10.00*G5)/(2.00*GM)
      X( 1)=-D
      X( 2)=-D/(2.00*TS)
      X( 3)=0.D0
      X( 4)=+D/T2
      X( 5)=2.00*D/T3
      X( 6)=-D2/2.00
      X( 7)=0.D0
      X( 8)=D2/(2.00*T2)
      X( 9)=D2/T3
      X(10)=-D3/3.00
      X(11)=0.D0
      X(12)=D3/(3.00*T2)
      X(13)=0.D0
      X(14)=D5/(5.00*T2)
      X(15)= 2.00*D5/(5.00*T3)
      X(16)=D6/(6.00*T2)
      X(17)=D7/(7.00*T2)
      X(18)=2.00*D7/(7.00*T3)
      X(19)=D8/(4.00*T3)
      X(20)=2.00*G1/T3
      X(21)=3.00*G1/T4
      X(22)=2.00*G2/T3
      X(23)=4.00*G2/T5
      X(24)=2.00*G3/T3
      X(25)=3.00*G3/T4
      X(26)=2.00*G4/T3
      X(27)=4.00*G4/T5
      X(28)=2.00*G5/T3
      X(29)=3.00*G5/T4
      X(30)=2.00*G6/T3
      X(31)=3.00*G6/T4
      X(32)=4.00*G6/T5
      IF(ID.GT.0)GO TO 402
      RETURN
  402 P=0
      DO 401 I=1,32
  401 P=P+G(I)*X(I)
      PP=P
```

```
      RETURN
      ENTRY DUDN
C     TERMS NEEDED FOR ENTHALPY CALCULATION
      K=5
      GO TO 1
  500 CONTINUE
C     H=H0+(T*DSDN(D)-DSDN(0))*101.325+(DUDN(D-DUDN(0))*101.325+CPOH(T)
C     +(P/D-R*T)*101.325
      G1=F/(2.00*GM)
      G2=(F*D2-2.00*G1)/(2.00*GM)
      G3=(F*D4-4.00*G2)/(2.00*GM)
      G4=(F*D6-6.00*G3)/(2.00*GM)
      G5=(F*D8-8.00*G4)/(2.00*GM)
      G6=(F*D10-10.00*G5)/(2.00*GM)
      X( 1)=D*T
      X( 2)=D*TS
      X( 3)=D
      X( 4)=D/T
      X( 5)=D/T2
      X( 6)=D2*T/2.00
      X( 7)=D2/2.00
      X( 8)=D2/(2.00*T)
      X( 9)=D2/(2.00*T2)
      X(10)=D3*T/3.00
      X(11)=D3/3.00
      X(12)=D3/(3.00*T)
      X(13)=D4/4.00
      X(14)=D5/(5.00*T)
      X(15)=D5/(5.00*T2)
      X(16)=D6/(6.00*T)
      X(17)=D7/(7.00*T)
      X(18)=D7/(7.00*T2)
      X(19)=D8/(8.00*T2)
      X(20)=G1/T2
      X(21)=G1/T3
      X(22)=G2/T2
      X(23)=G2/T4
      X(24)=G3/T2
      X(25)=G3/T3
      X(26)=G4/T2
      X(27)=G4/T4
      X(28)=G5/T2
      X(29)=G5/T3
      X(30)=G6/T2
      X(31)=G6/T3
      X(32)=G6/T4
      IF(ID.GT.0)GO TO 502
      RETURN
  502 P=0
      DO 501 I=1,32
  501 P=P+G(I)*X(I)
      PP=P
      RETURN
      ENTRY TDSDT
C     TEMP. TIMES THE PARTIAL OF
C     ENTROPY WITH RESPECT TO TEMP.
      K=6
      GO TO 1
  600 CONTINUE
C     CV=CV0+(TDSDN(/)-TDSDN(D))*101.325
      G1=F/(2.00*GM)
      G2=(F*D2-2.00*G1)/(2.00*GM)
      G3=(F*D4-4.00*G2)/(2.00*GM)
      G4=(F*D6-6.00*G3)/(2.00*GM)
      G5=(F*D8-8.00*G4)/(2.00*GM)
      G6=(F*D10-10.00*G5)/(2.00*GM)
      X(1)=0
      X( 2)=-D/(4.00*TS)
      X(3)=0
      X( 4)=2.00*D/T2
      X( 5)=6.00*D/T3
      X(6)=0
      X(7)=0
      X( 8)=D2/T2
      X( 9)=3.00*D2/T3
      X(10)=0
      X(11)=0
      X(12)=(2.00*D3)/(3.00*T2)
      X(13)=0
```

```
      X(14)=(2.00*D5)/(5.00*T2)
      X(15)=(6.00*D5)/(5.00*T3)
      X(16)=D6/(3.00*T2)
      X(17)=(2.00*D7)/(7.00*T2)
      X(18)=(6.00*D7)/(7.00*T3)
      X(19)=(3.00*D8)/(4.00*T3)
      X(20)=6.000*G1/T3
      X(21)=12.00*G1/T4
      X(22)=6.000*G2/T3
      X(23)=20.00*G2/T5
      X(24)=6.000*G3/T3
      X(25)=12.00*G3/T4
      X(26)=6.000*G4/T3
      X(27)=20.00*G4/T5
      X(28)=6.000*G5/T3
      X(29)=12.00*G5/T4
      X(30)=6.000*G6/T3
      X(31)=12.00*G6/T4
      X(32)=20.00*G6/T5
      IF(ID.GT.0)GO TO 602
      RETURN
  602 P=0
      DO 601 I=1,32
  601 P=P+G(I)*X(I)
      PP=P
      RETURN
      ENTRY DP2D2
C     SECOND PARTIAL OF PRESSURE WITH
C     RESPECT TO DENSITY SQUARED
      K=7
      GO TO 1
  700 CONTINUE
      F1=2.*F*GM*D
      F12=2.*F1*GM*D+2.*F*GM
      F212=3.*F1*D2+3.*2.*D*F+F12*D3+F1*3.*D2
      F222=5.*F1*D4 +5.*4.*D3*F+5.*D4*F1+F12*D5
      F232=7.*F1*D6+7.*6.*D5*F+7.*D6*F1+F12*D7
      F242=9.*F1*D8+9.*8.*D7*F+9.*D8*F1+F12*D9
      F252=11.*F1*D10+10.*11.*D9*F+11.*D10*F1+F12*D11
      F262=13.*F1*D12+13.*12.*D11*F+13.*D12*F1+F12*D13
      B(1)=2.*T   $B(2)=2.*TS   $   B(3)=2.
      B(4)=2./T   $   B(5)=2./T2   $   B(6)=6.*D*T
      B(7)=6.*D   $   B(8)=6.*D/T   $   B(9)=6.*D/T2
      B(10)=12.*D2*T   $   B(11)=12.*D2   $   B(12)=12.*D2/T
      B(13)=20.*D3   $   B(14)=30.*D4/T   $   B(15)=30.*D4/T2
      B(16)=42.*D5/T   $   B(17)=56.*D6/T   $   B(18)=56.*D6/T2
      B(19)=72.*D7/T2   $   B(20)=F212/T2   $   B(21)=F212/T3
      B(22)=F222/T2
      B(23)=F222/T4   $   B(24)=F232/T2   $   B(25)=F232/T3
      B(26)=F242/T2   $   B(27)=F242/T4   $   B(28)=F252/T2
      B(29)=F252/T3   $   B(30)=F262/T2   $   B(31)=F262/T3
      B(32)=F262/T4
      M=32
      IF(ID.GT.0)GO TO 702
      B(33)=PP
      RETURN
  702 P=0
      DO 701 I=1,M
  701 P=P+B(I)*G(I)
      PP=P
      RETURN
      END
```

```
      FUNCTION FIND D(P,T)
C     ITTERATES EQUATION OF STATE
C     FOR DENSITY, GIVEN PRESSURE
C     AND TEMP. IN ATM. AND KELVIN.  IF
C     ITTERATION FAILS TRY USING
C     FUNCTION CALLED FIND M
      COMMON/DATA/G,R,GAMMA,VP,DTP
      DIMENSION G(32),VP(9)
      TT=T
      PC=VPN(VP(8))
      IF(TT.GT.VP(8))GO TO 100
      IF( P.GT.VPN(TT))GO TO 101
      X=P*(.8-1.)/PC+1.0
      DD=P/(R*T*X)
      GO TO 102
  100 X=(1.1/(9.*PC))*P+.7/9.
      DD=P/(R*T*X)
      IF(P/PC.GT.20..AND.T/VP(8).LT.2.5)DD=DTP
      GO TO 102
  101 DD=DTP
  102 CONTINUE
      DO 10 I=1,50
      CALL PRESS(PP,DD,TT)
      P2=PP
      IF(ABS (P-P2)-1.E-7*P)20,20,1
    1 CALL DPDD(PP,DD,TT)
      DP=PP
      CORR=(P2-P)/DP
      D=DD
      IF(ABS (CORR)-1.E-7*D)20,20,10
   10 DD=DD-CORR
      FIND D=0
      RETURN
   20 FIND D=DD
      RETURN
      END
```

```
      FUNCTION FIND M(P,T,DD)
C     ALTERNATIVE FOR FIND D, INPUT IS
C     PRESSURE IN ATM., T IN KELVIN AND
C     DENSITY IN MOL/L.  INPUT DENSITY
C     IS A STARTING VALUE FOR ITTERATION
C     OF EQUATION OF STATE FOR SOLUTION FOR P AND T
      TT=T
      DO 10 I=1,50
      CALL PRESS(PP,DD,TT)
      P2=PP
      IF(ABS (P-P2)-1.E-7*P)20,20,1
    1 CALL DPDD(PP,DD,TT)
      DP=PP
      CORR=(P2-P)/DP
      D=DD
      IF(ABS (CORR)-1.E-7*D)20,20,10
   10 DD=DD-CORR
      FIND M=0
      RETURN
   20 FIND M=DD
      RETURN
      END
```

```
      FUNCTION ENTHAL(P,D,T)
C     CALCULATES ENTHALPY FOR INPUT OF
CC    PRESSURE, DENSITY AND TEMP. IN
CC    ATM., MOL/L AND K.  OUTPUT IS IN
C     JOULES/MOL
      R=.08205616
      DD=D
      TT=T
      CALL DSDN(SD,DD,TT)
      CALL DUDN(UD,DD,TT)
      DD=0
      CALL DSDN(S0,DD,TT)
      CALL DUDN(U0,DD,TT)
      ENTHAL=T*(SD-S0)*101.325+(UD-U0)*101.325+HI(T)+(P/D-R*T)*101.325
      RETURN
      END



      FUNCTION ENTROP(D,T)
C     CALCULATES ENTROPY
CC    FOR AN INPUT OF DENSITY AND
CC    TEMP. IN MOL/L AND K.  OUTPUT IS IN
C     JOULES/MOL-K
      R=.08205616
      DD=D
      TT=T
      CALL DSDN(SD,DD,TT)
      DD=0
      CALL DSDN(S0,DD,TT)
      ENTROP=(SD-S0)*101.325-R*ALOG(D*R*T)*101.325+SI(T)
      RETURN
      END



      FUNCTION SOUND(D,T)
C     CALCULATES THE SPEED OF SOUND
CC    FOR AN INPUT OF DENSITY AND TEMP.
CC    IN MOL/L AND KELVIN.  OUTPUT IS IN
C     METERS/SECOND.
      COMMON/CRIT/W
      CALL DPDD(DP,D,T)
      SOUND=((CP(D,T)/CV(D,T))*DP*101325./W)**.5
      RETURN
      END



      FUNCTION CP(D,T)
C     CALCULATES SPECIFIC HEAT CAPACITY
CC    AT CONSTANT PRESSURE FOR INPUT OF
CC    DENSITY AND TEMPERATURE IN MOL/L AND K
C     CP IS IN JOULES/MOL-K
      CVEE=CV(D,T)
      CALL DPDT(DPT,D,T)
      CALL DPDD(DPD,D,T)
      CP=CVEE+(T/(D**2)*(DPT**2)/DPD)*101.325
      RETURN
      END
```

```
      FUNCTION CV(D,T)
C     CALCULATES SPECIFIC HEAT CAPACITY
C     AT CONSTANT VOLUME FOR AN INPUT
C     OF DENSITY AND TEMPERATURE IN MOL/L AND K
      DATA(R=8.314434)
      DD=D
      TT=T
      CALL TDSOT(CD,DD,TT)
      DD=0
      CALL TDSOT(C0,DD,TT)
      CV=CPI(TT)+(C0-CD)*101.325
      CV=CV-R
      RETURN
      END
```

```
      FUNCTION CPI(T)
C     CALCULATES IDEAL GAS THERMO PROPERTIES
C     FOR ALL FLUIDS EXCEPT H2.  INPUT IS IN
C     KELVIN, OUTPUT IS IN JOULES, MOL/L AND K
      COMMON/CPID/G(11)
      COMMON/ISP/N
      K=1
    1 U=G(9)/T
      EU=EXP (U)
      TS=1./T**4
      GO TO (2,3,4),K
    2 CPI=G(8)*U*U*EU/(EU-1.)**2
      DO 10 I=1,7
      TS=TS*T
   10 CPI=CPI+G(I)*TS
      CPI=CPI*8.31434
      RETURN
      ENTRY SI
      K=2
      GO TO 1
    3 CPI=G(8)*(U/(EU-1.)-ALOG(1.-1./EU))
     1-G(1)*TS*T/3.-G(2)*TS*T*T/2.-G(3)/T+G(4)*ALOG(T)+G(5)*T+G(6)*T*T/2
     2.+G(7)*T**3/3.
      CPI=CPI*8.31434+G (11)
      RETURN
      ENTRY HI
      K=3
      GO TO 1
    4 CPI=G(8)*U*T/(EU-1.)-G(1)/(2.*T*T)-G(2)/T+G(3)*ALOG(T)+G(4)*T
     1+G(5)*T*T/2.+G(6)*T**3/3.+G(7)*T**4/4.
      CPI=CPI*8.31434+G(10)
      RETURN
      END
```

```
      FUNCTION VISC(DD,T)
C     RETURNS VISCOSITY IN (G/CM-S)*E+6,
C     T IN K, D IN MOL/L
      COMMON/CRIT/EM
      D=DD*EM/1000.
      VISC=DILV(T)+FDCV(D,T)+EXCESV(D,T)
      RETURN
      END



      FUNCTION DILV(T)
C     GIVES DILUTE GAS VISCOSITY AND THERMAL
C     CONDUCTIVITY FOR AN INPUT TEMP. IN
C     KELVIN.  OUTPUT UNITS ARE SAME AS
C     THOSE IN VISC AND THERM
      COMMON/ISP/N,NW,NWW
      COMMON/DATA1/GV,GT,FV,FT,EV,ET
      DIMENSION GV(9),GT(9),FV(4),FT(4),EV(8),ET(8)
      SUM=0
      TF=T**(1./3.)
      TFF=T**(-4./3.)
      DO 10 I=1,9
      TFF=TFF*TF
   10 SUM=SUM+GV(I)*TFF
      IF(NWW.EQ.7) GO TO 9
      DILV=SUM*1000.
      GO TO 11
    9 DILV=SUM
   11 RETURN
      ENTRY DILT
      TF=T**(1./3.)
      TFF=T**(-4./3.)
      SUM=0
      DO 20 I=1,9
      TFF=TFF*TF
   20 SUM=SUM+GT(I)*TFF
      DILV=SUM
      RETURN
      END



      FUNCTION FDCV(D,T)
C     FIRST DENSITY CORRECTION
C     FOR VISCOSITY AND THERMAL CONDUCTIVITY
      COMMON/DATA1/GV,GT,FV,FT,EV,ET
      DIMENSION GV(9),GT(9),FV(4),FT(4),EV(8),ET(8)
      FDCV=(FV(1)+FV(2)*(FV(3)-ALOG(T/FV(4)))**2)*D
      RETURN
      ENTRY FDCT
      FDCV=(FT(1)+FT(2)*(FT(3)-ALOG(T/FT(4)))**2)*D
      RETURN
      END
```

```
      FUNCTION EXCESV(D,T)
C     CALCULATES EXCESS VISCOSITY
      COMMON/DATA1/GV,GT,FV,FT,EV,ET
      COMMON/ISP/N,NW
      DIMENSION GV(9),GT(9),FV(4),FT(4),EV(8),ET(8)
      R2=D**(.5)*((D-EV(8))/EV(8))
      R=D**(.1)
      X=EV(1)+EV(2)*R2+EV(3)*R+EV(4)*R2/(T*T)+EV(5)*R/T**(1.5)+EV(6)/T
     1+EV(7)*R2/T
      X1=EV(1)+EV(6)/T
      EXCESV=EXP (X)-EXP (X1)
      RETURN
      ENTRY EXCEST
C     CALCULATES EXCESS THERMAL CONDUCTIVITY
       IF(NW.EQ.0 ) GO TO 3
      R=D**(.1)
      X=ET(1)+ET(2)*R+ET(3)*R/T**(1.5)+ET(4)/T
      X1=ET(1)+ET(4)/T
      EXCESV=(EXP (X)-EXP (X1))/10.
      RETURN
    3 R2=D**(.5)*((D-ET(8))/ET(8))
      R=D**(.1)
      X=ET(1)+ET(2)*R2+ET(3)*R+ET(4)*R2/(T*T)+ET(5)*R/T**(1.5)+ET(6)/T
     1+ET(7)*R2/T
      X1=ET(1)+ET(6)/T
      EXCESV=EXP (X)-EXP (X1)
      RETURN
      END


      FUNCTION THERM(DD,T)
C     RETURNS TC IN MW/M-K, T IN K, D IN MOL/L
      COMMON/HAN/CR,TCI
      COMMON/ISP/N,NW
      COMMON/CRIT/EM
      D=DD*EM/1000.
      IF(NW.EQ.0 ) GO TO 3
      CR=CRITC(D,T)
      THER=DILT(T)+FDCT(D,T)*100.+EXCEST(D,T)+CR
      TCI=THER-CR
       THERM=THER
      RETURN
    3 CR=CRITC(D,T)
      THERM=DILT(T)+FDCT(D,T)+EXCEST(D,T)+CR
      TCI=THERM-CR
      RETURN
      END


      FUNCTION SENG(D,T)
C     SCALED EQUATION OF STATE FOR CRITICAL REGION
      COMMON/CRIT/ EM, EOK, RM, TC, DC, X , PC, SIG
      COMMON/SEN/BETA,XO,DELTA,E1, E2, AGAM
      COMMON/CHECK/DELD,DELT,DSTAR,TSTAR
      DSTAR= D/DC $ TSTAR=T/TC
      BETO=1./BETA
      XX=DELT/DELD**BETO
      AG=AGAM-1.0
       BET2= 2.0*BETA
      AGB=AG/BET2
      DEL1=DELTA-1.0
       AGBB=(AG-BET2)/BET2
      XXO=(XX+ XO)/XO
      XXB=XXO**BET2
      BRAK=1.0 + E2*XXB
       BRAK1=BRAK**AGB
      H=E1*XXO*BRAK1
      HPRIM=(E1/XO)*BRAK1 + (AG/XO)*E1*E2*(XXB)*(BRAK**AGBB)
      RCOM=(DELD**DEL1)*(DELTA*H - (XX/BETA)*HPRIM  )
      RCOMP=1.0/(RCOM*DSTAR**2)
      RCM=RCOMP/(PC*1.01325E+06)
C    RCM IN DYNES
      RCM=RCM**0.5
C
       SENG=RCM
       RETURN
       END
```

```
      FUNCTION CRITC(D,T)
C     CALCULATES CRITICAL ENHANCEMENT
C     FOR THERMAL CONDUCTIVITY
      COMMON/CRIT/ EM, EOK, RM, TC, DC, X , PC, SIG
      COMMON/CHECK/DELD,DELT,DSTAR,TSTAR
      COMMON/HJM/EPSI,CPCV,RRR,AKT
      COMMON/ISP/N,NW,NWW
C D IN G/CM3 , T IN K
C  OUTPUT UNITS ARE MW/M.K
      AV=6.0225E+23 $ BK=1.38054E-16
       DELD=ABS ((D-DC)/DC $ DELT=ABS (T-TC)/TC
C  CALCULATE DISTANCE PARAMETER
      R=(RM**2.5)*(D**0.5)*(AV/EM)**0.5
      R=R*(EOK**0.5)*X/(T**0.5)
      RRR=R
C   GENERAL  EQUATION
      DX=D*1000.0/EM
      CALL DPDT(DPT,DX,T)
C  DPDT  IN  ATS PER DEG.
      DPT=DPT*1.01325E+6
C  DPDT NOW IN DYNES PRR DEG
      CALL DPDD(DPD,DX,T)
C  DPDD UN ATS, MOL/L
      DPD=DPD*(1.01325E+6)*(1000.0/EM)
CDPDD NOW IN DYNES, GM/CM3
      IF( DPD.LT.0.0) DPD=1.0
   94 VIS=VISC(DX,T)*(1.0E-06)
C   VISCOSITY IN GM/CM.S
      IF(DELD.EQ.0.25. OR. DELD.LT. 0.25) 8,10
    8 IF(DELT.EQ.0.025. OR. DELT.LT.0.025 ) 9, 10
    9 COMPRES=SENG(D,T)
      GO TO 12
   10 COMPRES=1.0/(D*DPD)**0.5
   12 EX=BK*T**2*(DPT**2)*COMPRES
      EXB=R*((BK*T)**0.5)*(D**0.5)*((AV/EM)**0.5)
      CRIT=EX/(EXB*6.0*3.14159*VIS)
C   PUT IN DAMPING FACTOR
      BDD=((D-DC)/DC)**4
      BTT=((T-TC)/TC)**2
      FACT=EXP (-18.66*BTT - 4.25*BDD)
      DELC=CRIT*FACT/100.0
      CRITC=DELC
       AKT=COMPRES*COMPRES
      EPSI=R*R*BK*T*(AV*D/EM)*AKT
      EPSI=EPSI**0.5
C   CALC  CP-CV
      CPCV=T*(DPT**2)*AKT/D
      RETURN
       END
```

```
      PROGRAM VALUES(OUTPUT,INPUT)
      CALL DATA 02
      PRINT 20
   20 FORMAT(82H1     P              T            RHO                H              S
     1     C-V          C-P        VEL/82H      ATM          KELVIN        MOL/L
     2    J/MOL     J/MOL-K    J/MOL-K    J/MOL-K   M/SEC/1H )
      DO 19 I=1,5
    4 READ 5,P,T
    5 FORMAT(F9.3,F8.3)
      DEN=FINDD(P,T)
      H=ENTHAL(P,DEN,T)
      S=ENTROP(DEN,T)
      CVE=CV(DEN,T)
      CPE=CP(DEN,T)
      VEL=SOUND(DEN,T)
      PRINT 13,P,T,DEN,H,S,CVE,CPE,VEL
   13 FORMAT(F10.4,F12.5,F10.6,F12.1,3F10.2,F8.0)
   19 CONTINUE
      END
```

P ATM	T KELVIN	RHO MOL/L	H J/MOL	S J/MOL-K	C-V J/MOL-K	C-P J/MOL-K	VEL M/SEC
50.0000	60.00000	40.237637	-5780.0	71.95	35.00	53.16	1127.
50.0000	100.00000	35.252617	-3480.5	97.93	29.39	52.58	902.
.40.0000	200.00000	13.500484	3013.2	141.86	24.63	71.41	295.
00.0000	200.00000	22.282750	2062.6	132.73	24.40	54.66	497.
00.0000	300.00000	24.548716	6948.2	140.30	24.72	40.42	738.

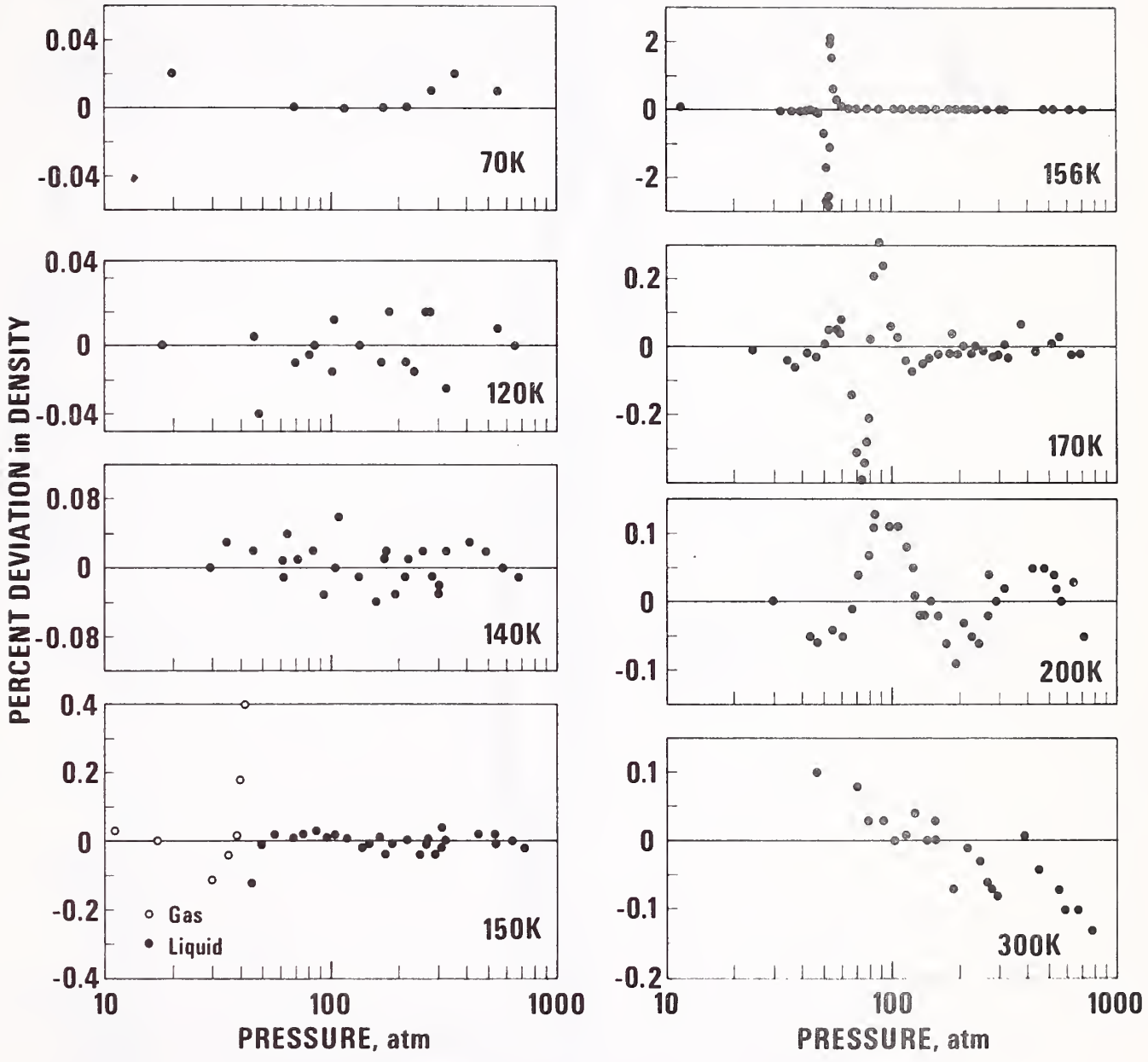

Figure 1. Deviations of the density data from eqn. (1) on several isotherms.

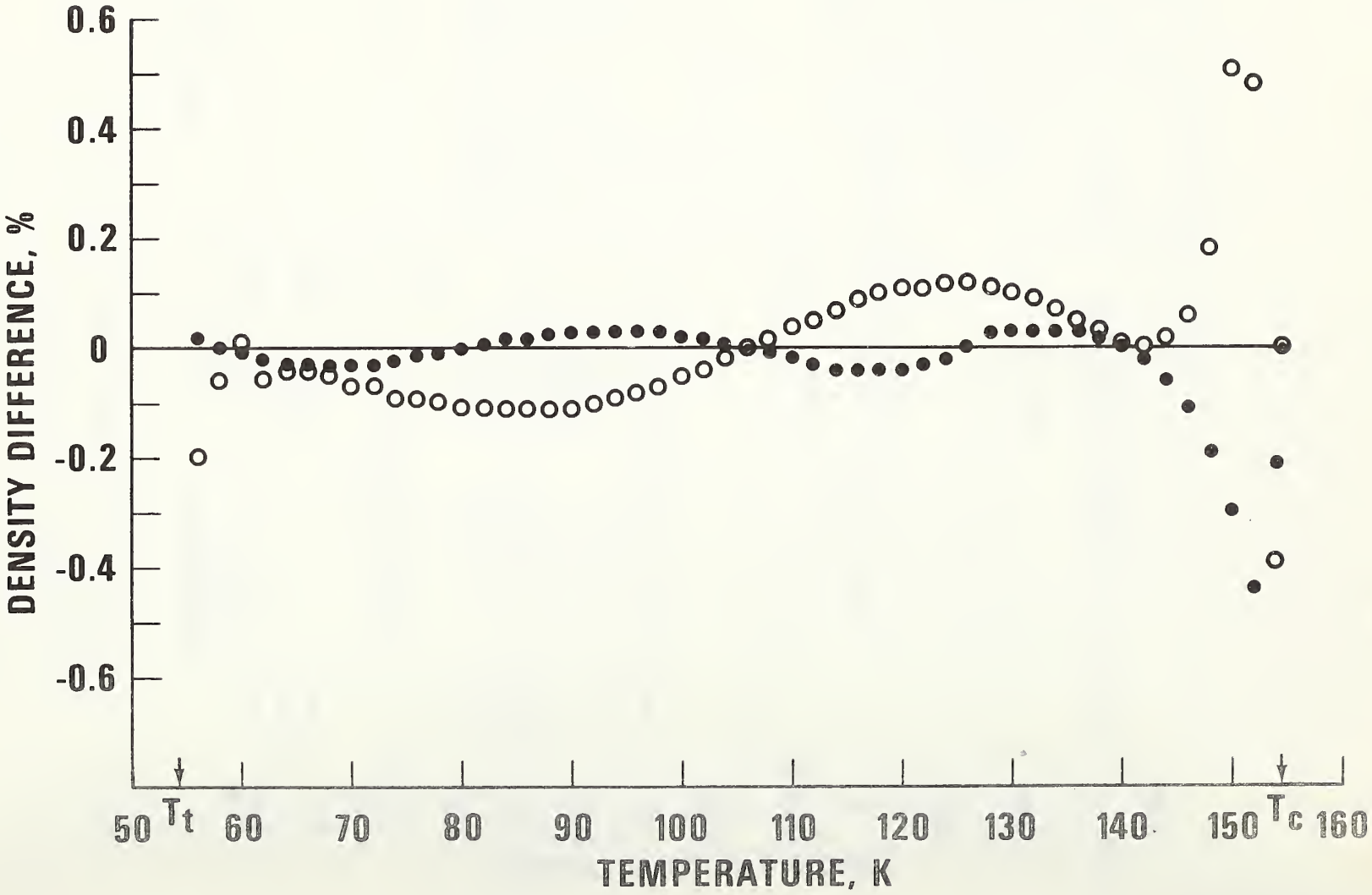

Figure 2. Deviations of the saturation densities from the values calculated via eqn. (1); O - liquid, O - vapor.

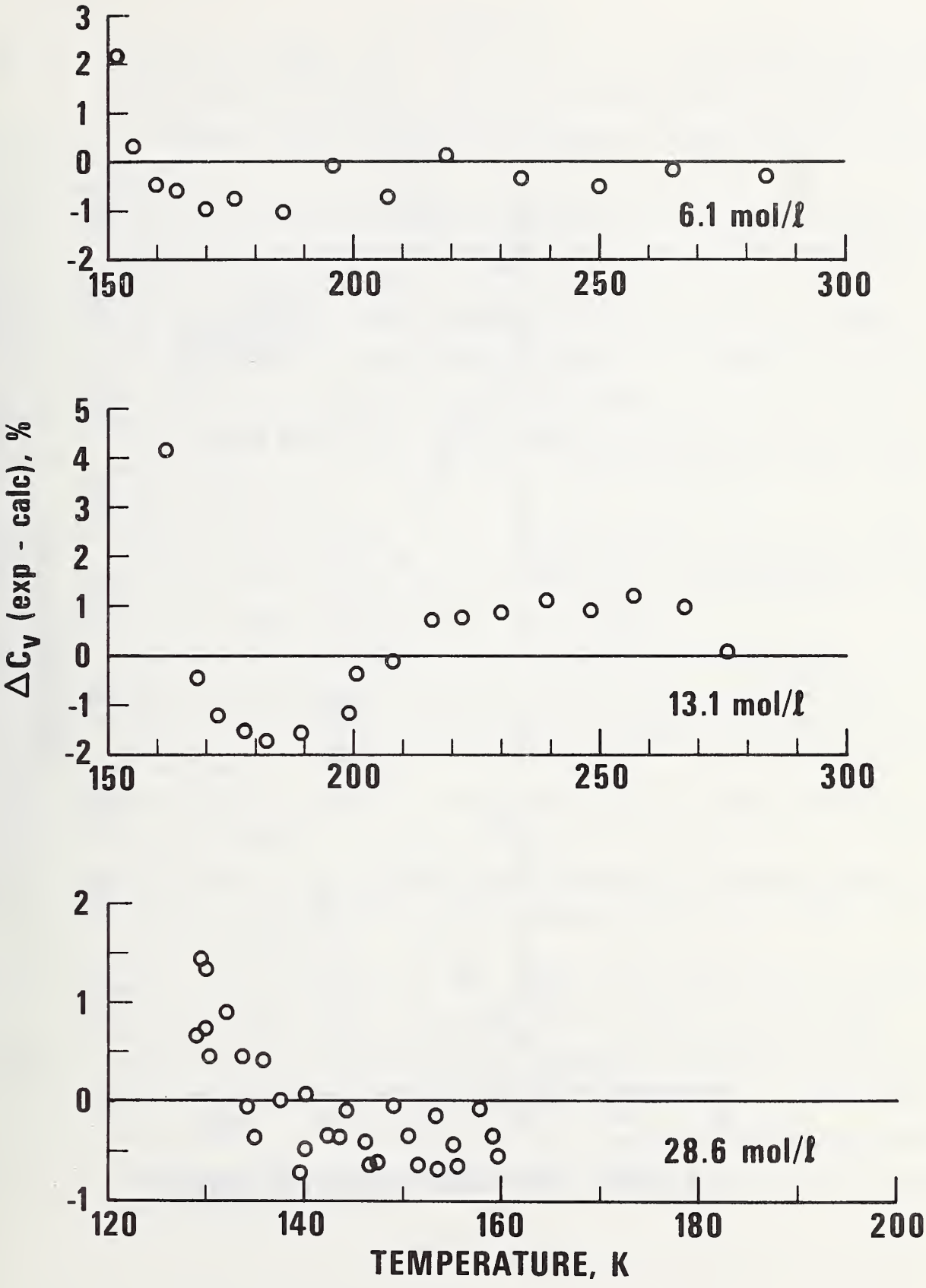

Figure 3. Deviations of the heat capacity data on three isochores from values calculated by eqn. (1).

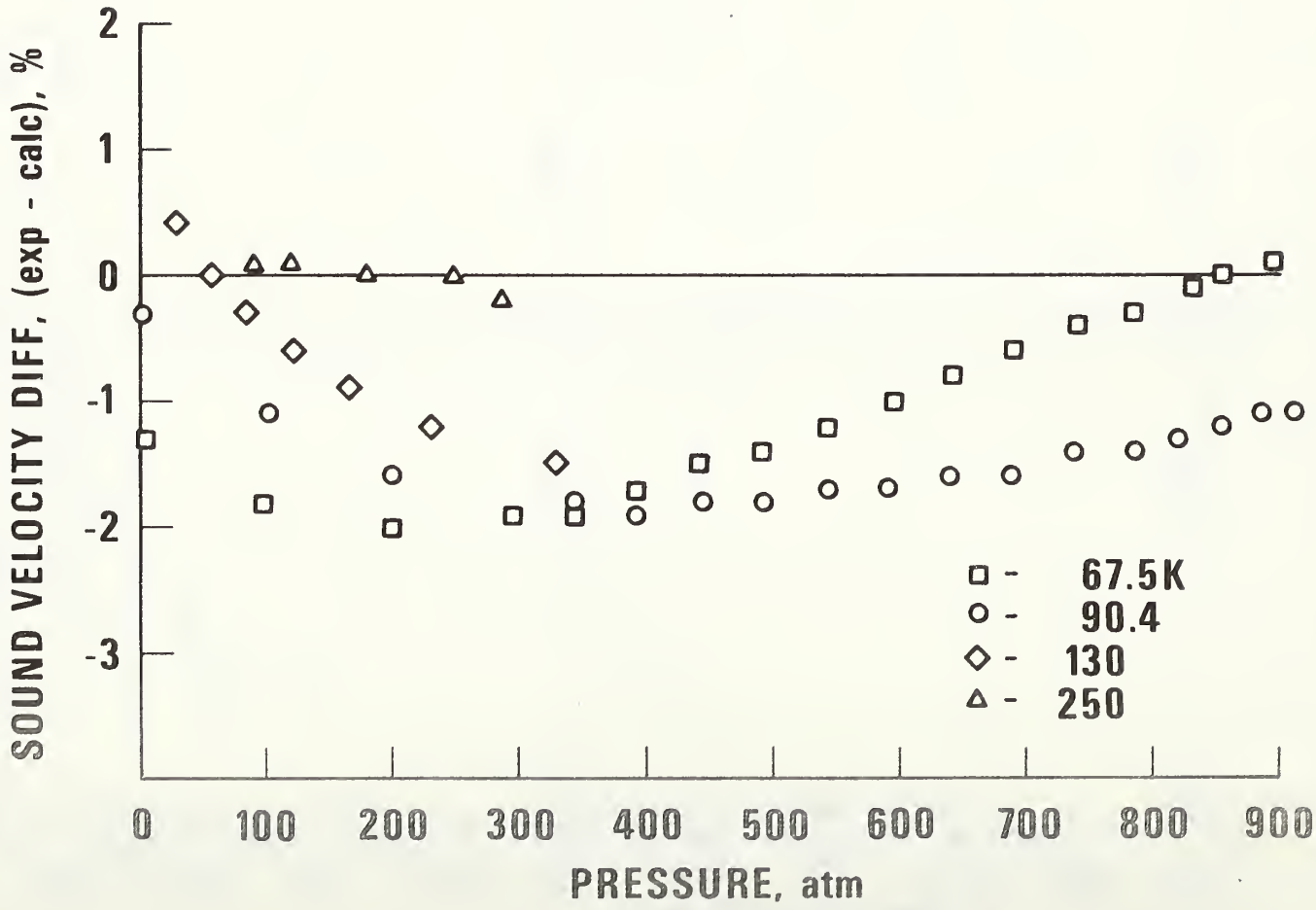

Figure 4. Deviations of the velocity of sound data from values calculated via the equation of state on several isotherms.

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16. ABSTRACT *(A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here.)*

New PVT data on oxygen at pressures to 800 atmospheres have been recently reported. These data, along with other NBS data on oxygen, have been fitted with a 32 term modified Benedict-Webb-Rubin equation of state. This equation is valid for gaseous and liquid oxygen at temperatures from the triple point (54.36 K) to 300 K and for pressures up to 800 atm. Thermophysical properties calculated via this equation are compared with the most reliable values available. The vapor pressure equation has also been updated to be consistent with more recent experimental work near the triple point. A computer program is available which calculates the thermophysical properties of oxygen.

17. KEY WORDS *(six to twelve entries; alphabetical order; capitalize only the first letter of the first key word unless a proper name; separated by semicolons)*

Density; enthalpy; entropy; equation of state; oxygen; property computer program; PVT; saturation properties; specific heat.

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